

chain nodes:

25 26 27 28 29 30

ring nodes:

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24

chain bonds:

2-28 5-9 12-14 17-21 24-25 25-26 26-27 28-29 29-30

ring bonds:

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15 15-16 16-17 17-18 19-20 19-24 20-21 21-22 22-23 23-24

exact/norm bonds:

2-28 24-25

exact bonds:

5-9 12-14 17-21 25-26 26-27 28-29 29-30

normalized bonds:

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15 15-16 16-17 17-18 19-20 19-24 20-21 21-22 22-23 23-24

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:CLAS\$26:CLAS\$27:CLAS\$28:CLAS\$29:CLAS\$30:CLAS\$

C:\Program Files\Stnexp\Queries\531376y.str

$$\mathbf{g} = \left[\mathbf{c} \mathbf{g} \right]_{0-12} \left[\mathbf{c} \mathbf{g} \right]_{0-1}$$

chain nodes:

19 22 23 24

ring nodes:

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18

chain bonds:

2-22 5-9 12-14 17-19 22-23 23-24

ring bonds:

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15 15-16 16-17 17-18

exact/norm bonds:

1-2 1-6 2-3 2-22 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 17-19

exact bonds:

5-9 12-14 22-23 23-24

normalized bonds:

13-14 13-18 14-15 15-16 16-17 17-18

G1:CI,F,CN

G2:C,O

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLAS\$22:CLAS\$23:CLAS\$24:CLAS\$